

Toluene
108-88-3 | DTXSID7021360

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 9.74e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.74e-01

Confidence level: 9.04e-01

Nearest Neighbors from the Training Set

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1,3,5-Cycloheptatriene

Measured: 9.69e-11

Predicted: 1.00e-10

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Cyclohepta-1,3-diene

Measured: 1.39e-10

Predicted: 1.35e-10

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1,4-Cyclohexadiene

Measured: 1.00e-10

Predicted: 1.11e-10

Image not found

(E)-Crotonaldehyde

Measured: 3.61e-11

Predicted: 3.73e-11

Image not found

Crotonaldehyde

Measured: 3.61e-11

Predicted: 3.73e-11